Field controllable polymer hybrids in action

Drs Marina Saphiannikova-Grenzer, **Olga Guskova**, **Vladimir Toshchevikov** and **Dmytro Ivaneyko** from the Material Theory and Modelling group research functional polymer materials for a wide range of applications. Here, they expand on their activities

Can you begin by describing the work your group does and the foci of your research?

MG: Our group has complementary scientific backgrounds in the fields of theoretical chemistry, theoretical physics and material engineering, with an emphasis on small organic molecules and polymers. However, our current research interests are not limited to pure organic materials. In recent years, our research into polymer hybrids has increased; they have gained tremendous scientific and industrial attention owing to their unique properties. These materials synergistically combine the best features from inorganic, organic and even biological worlds.

Importantly, the behaviour of polymer hybrids can be remotely controlled by the light and magnetic fields, which makes them especially attractive for a modern society. Our target is to understand and predict how the structure of these field controllable hybrids defines their macroscopic properties. Our dream is to be able to assist the manufacture of diverse polymer hybrids according to customer specifications and the needs of society.

What kinds of applications does your research on functional polymer materials have?

VT&OG: The fields of our scientific interests include hybrid materials of various structures, whose components define their physical properties and specific applications. One of our research activities is devoted to magneto-sensitive elastomers. These have found practical applications in controllable membranes, rapid-response interfaces designed to optimise mechanical systems, and in automobile applications, such as adaptive-tuned vibration absorbers, stiffness tuneable mounts and bushings, and automobile suspensions.

Other scientific activities are devoted to azobenzene-containing polymer hybrids, which have fascinating potential for applications as sensors, actuators, microrobots, micropumps, artificial muscles for exoskeletons and robots. Last but not least, we predict the behaviour of polymers for organic electronics when they are in contact with another material or interface. This topic is of particular interest for further development of energy-efficient devices.

Can you tell us what you find most interesting about magneto-sensitive elastomers (MSEs)?

DI: MSEs are viscoelastic polymer composites with inclusions of ferromagnetic particles. They exhibit unique mechanical properties under external magnetic fields that are the result of a synergy between elastic and magnetic components. One of the most fascinating features of MSEs is the change of the mechanical moduli under an applied magnetic field, as well as the ability to generate magnetically induced deformations and actuation stresses. The mechanical properties of MSEs strongly depend on the elasticity of the polymer matrix, volume concentration of the particles, and their shape, size and spatial distribution. Because of their unique properties, MSEs are of strong commercial interest in numerous fields, from automotive to medicine to soft robotics. Several industrial groups already incorporate MSEs into their devices.

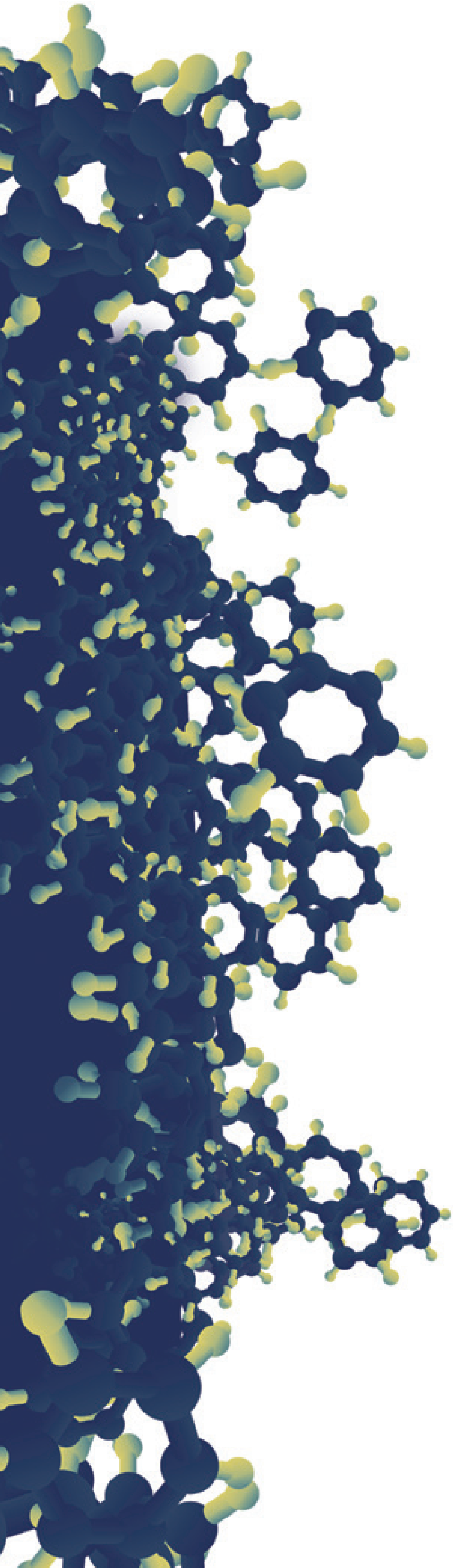
How do you overcome the particular challenges you face in your research?

VT&MG: The theoretical description of the structure and dynamics of polymer hybrids inside a broad range of time and length scales is an extremely challenging task. It would be impossible to solve it if all the details and processes were simultaneously taken into account. We use our expertise to identify key details that influence the macroscopic properties of interest and issue appropriate material models. In particular, we use the powerful tools of coarse-graining and renormalisation to describe the physical properties of the materials on specific scales, ranging from nanometres to centimetres. Unifying all key physical processes into one picture, we obtain a multiscale approach that is able to describe physical properties of the material in a broad range of time and length scales.

Could you reveal any future plans for the group?

MG: In its present state, our international group consists mainly of early- and mid-career researchers whose primary ambition is to become leading experts on the scientific market in the aforementioned fields of research. This demands stable income from funding agencies, so the nearest future plans presume securing of long-term financial support by getting prestigious research grants in close collaboration with experimentalists and industrial firms.

This will allow us to employ additional personnel and strengthen our efforts to meet research goals. The personal strategic plans include acquisition of the next scientific and academic degrees by the group members, as well as the department status of the group. For strategic research initiatives, we would like to build and maintain a successful research network with industrial partners in areas alluded to above.



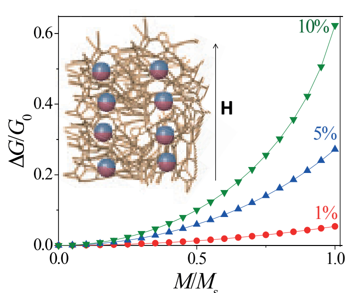
From fundamental science through to R&D

Researchers at the **Leibniz Institute of Polymer Research Dresden** are working to advance knowledge regarding the development of field controllable polymer hybrids with new and improved characteristics. Their findings will enable the production of new materials with diverse practical applications

Drs Vladimir Toshchevikov, Olga Guskova, Marina Grenzer and Dmytro Ivaneyko

FIELD CONTROLLABLE POLYMER hybrids are multicomponent materials made up of a polymer matrix with organic or inorganic additives. The polymer component, as German chemist Hermann Staudinger understood back in 1920, is represented by giant chain-like macromolecules built from repeating chemical units bonded together. Polymers boast a wide range of mechanical and physical properties, but as such lack sensitivity to external electric, magnetic and light fields. This can be outsmarted in polymer hybrids by incorporating light-sensitive moieties or iron particles in otherwise non-conductive and non-magnetic polymers. The resulting polymer hybrids show a strong response to external fields and can be controlled by the latter.

The breadth of potential for the polymer hybrids is such that they present a fascinating and exciting field of enquiry in both science and technology. Indeed, field controllable polymers are one example of polymers that have been created with an extraordinary amount of advanced magnetic, optic and electronic properties. The benefits of research into this specific type of polymer includes the fact that it is possible to tweak the properties of it without exorbitant cost. Material usage is also often low which, given the ever-increasing environmental concerns, is a particularly attractive perspective.



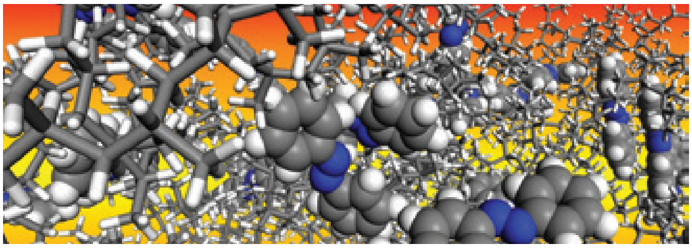
Relative change of the shear modulus of MSEs as a function of the relative magnetisation for different volume fractions of particles: 1%, 5% and 10%.

The 'Material Theory and Modelling' (MTM) group focuses on developing understanding of functional polymer materials that is orientated around practical applications. Together, Drs Marina Grenzer, Olga Guskova, Vladimir Toshchevikov and Dmytro Ivaneyko perform research into field controllable polymer hybrids. Their work represents the potential for imbuing materials with new field controllable functions that meet the demands of industry. The MTM group also researches mechanical behaviour of polymer networks reinforced with rigid particles, which is important for the development of tyres.

APPRECIATING REPRESENTATIONS FROM DIFFERENT SCALES

Theoretical studies on field controllable polymer hybrids is a rapidly growing field of polymer science that has been developing over the past few decades. Nowadays, it incorporates a number of novel theories and computer simulations to enable molecular and morphological designs, and predictions of macroscopic properties. As such, the MTM group performs computer simulations alongside analytical studies to generate deeper understanding of the molecular processes that occur in functional polymer hybrids under external fields.

"For our research, we apply a number of methods and approaches, including analytical models of statistical physics based on the



Polymer macromolecules with azobenzene chromophores (moieties with two aromatic rings) in side chains.

analysis of free energy and the dynamic Langevin equation," explains Grenzer. "We also take quantum chemical approaches and particle-based computer simulation techniques, like coarse-grained and full-atomistic molecular dynamics." The team's unique combination of expertise across the theoretical materials science field enables them to understand the structure and dynamics of field controllable materials on different time and length scales. "It is similar to making a film about the Black Forest," she says. "You need to use quite a number of different magnifiers to admire the forest in all its complexity. Similarly, we construct a multiscale picture of a particular field controllable material from representations of the material structure and physical processes taken across different scales."

Importantly, the multiscale approach developed by the team provides a deep understanding of the molecular processes and their relation with macro-properties of functional materials. The high predictive power of the team's multiscale approach can be used to guide the manufacturing of field controllable polymer materials for target practical applications.

MANY PARTS MAKE LIGHT WORK

Throughout the course of their studies, the team has developed further understanding of several field controllable polymers. Azobenzene-based hybrid materials have unique physical properties, can change their shape under illumination, and have been the subject of intense study for a number of years. The MTM group has developed an analytical theory to describe the photomechanical properties of these azobenzene polymers as a function of their chemical architecture. "The established structure-property relationships can be used by engineers of specific photo-deformable materials for specific applications," explains Toshchevikov.

ELASTIC POLYMER AND MAGNETIC PARTICLES: A PERFECT MARRIAGE

Another notable achievement of the MTM group is their work on magneto-sensitive elastomers (MSEs). These polymers are able to change their shape and mechanical behaviour under external magnetic fields. The team's unique theoretical approach not only describes the deformation and static moduli of MSEs, but also the dynamic moduli of these materials. As it stands, there are no other theoretical works to describe the field controllable dynamic moduli of MSEs. "The dynamic moduli characterise mechanical response of materials on oscillating mechanical stress and are important characteristics for design of elements affected by external oscillating loadings in practical applications," explains Ivaneyko. The approach the team has developed is particularly useful for those in the automobile industry who produce materials with field controllable stiffness for movable elements.

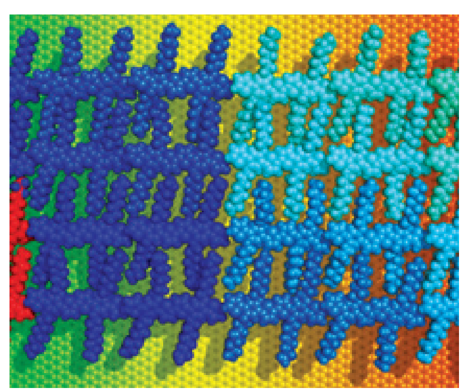
POLYMER HYBRIDS FOR AN ELECTRONIC WORLD

In today's world, in which every aspect of life is impacted by electronic technology, the development of required materials begins with computational design. New chemical structures, component combinations, and even the morphology of working units of devices like smartphone displays (based on polymer light-emitting diodes), photovoltaic cells and polymer field effect transistors can be predicted theoretically. "For instance, our simulations shed light on the controlled self-assembly of organic electronic molecules into arranged carpets at different interfaces, whose structure finally defines the performance of handheld or household gadgets," explains Guskova.

PERSPECTIVES: A LEAP FROM THEORY TO MANUFACTURING

The work of the MTM team is increasingly necessary to effectively guide the manufacturing of functional polymer materials with tailored properties. Their advanced research into field controllable hybrids gains rapidly in importance; as the structure of these fascinating materials can be smartly manipulated to perform a near-limitless amount of functions. This boasts huge potential for incorporating theoretical studies into the development of new products for a diverse range of practical applications.

There is a natural process to the research of the MTM team; their findings must take a leap from the theory and modelling stage through to manufacturing. As such, the members of MTM are keen to work with R&D professionals around the world to make the best use of their work on field controllable polymer hybrids. Similar to how there are multiple components to a successful marriage, the manufacturing of beneficial polymer hybrids will not be realised without the cooperation of partners from across academia and industry. The MTM team believes that one important component of this 'acting together' is a theoretical prediction of a field controlled response.



Organic electronic carpet on graphite solid surface

MATERIAL THEORY AND MODELLING (MTM) GROUP

OBJECTIVE

To develop an understanding of functional polymer materials that is orientated around practical applications.

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PD DR HABIL MARINA GRENZER graduated from St Petersburg State University (SPBU). In 1995, she received her PhD from the Institute of Macromolecular Compounds St Petersburg, IMC, and completed her habilitation in 2007 at the University of Potsdam. She currently leads the MTM group at IPF and is Associate Professor at TU Dresden.

OLGA GUSKOVA received her PhD from Ulm University, Germany, in 2008. She was a postdoc at the Max-Planck Institute of Colloids and Interfaces, Potsdam, Germany. In 2011, she joined IPF as research associate and, since 2015, has been a Junior Group Leader of Material Properties of Semi-Conducting Polymers.

DR VLADIMIR TOSHCHEVIKOV received his Master Degree in physics from SPBU in 1998 and, in 2002, defended his PhD thesis at IMC. At IMC, he had a longstanding collaboration with the Physical Institute, University of Freiburg, Germany. Presently he is research associate at IPF.